1. Parameter Settings for the Simulation of a Typical Cough

The transmission medium of the cough is modeled as an incompressible ideal gas with constant properties calculated at ambient conditions. The flow field evolution of coughing is time-dependent, so the simulations are conducted under a transient condition. Since the droplet volume fraction is very low in the cough flow, the Eulerian-Lagrangian method is used in this paper: 1) The continuous phase (the flow field) is modeled by the Eulerian method, which is to solve the Navier-Stokes equations; 2) The discrete phase (the droplet) is modeled by the Lagrangian method, i.e., by tracking the motion of the droplets; 3) The discrete phase can exchange mass, momentum, and energy with the continuous phase, thus fully considering the influence of the flow field on particle diffusion.

The renormalization group (RNG) k-ε model with scalable wall functions is selected as the turbulence model, and the discrete phase model is used for the droplet diffusion (Aliabadi et al., 2010; Gao and Niu, 2006; Zhang and Li, 2012; Zhang et al., 2017). Meanwhile, the transport model between components is used. In the discrete phase model, unsteady particle tracking is selected, and the particle time step size is 1×10^{-3} s. For tracking parameters, the max number of steps is 50,000, and the step length factor is 5. In physical methods, two-way turbulence coupling, stochastic collision, break-up, and coalescence are picked.

Due to the differences in measurement methods and the physiological variability of different volunteers, the size distribution of the droplets discharged from a cough is not unique (Chao et al., 2009). We use the droplet size distribution from (Chao et al., 2009; Duguid, 1946), and the population is modeled by fitting the data with a Rosin-Rammler distribution. The droplet group is injected in the time range of 4.20×10^{-2} s to 1.36×10^{-1} s with a temperature of 35 ℃. The injection speed is zero, and all droplets are driven initially by the flow field from the mouth (Borro et al., 2021). We pick the spherical drag model and consider the effect of secondary break-up through a Taylor Analogy Breakup model. Then, the Discrete Random Walk model is used to consider the effects of the turbulent flow on the droplets (Bi, 2018). Moreover, each droplet consists of multi-components (Aliabadi et al., 2010): 1) 94% volume fraction of the pure water which can be evaporated during the transmission, and 2) 6% volume fraction of the pure water but non-evaporative, which represents the mucus and physiological electrolytes that carry infectious agents. The boundary condition of the inlet is defined to be a velocity-inlet, and the velocity direction is set as normal to the boundary. The fluid injected from the inlet consists of air and water vapor at 35 ℃, with the mole fraction 93.80% and 6.20%, respectively (Bi, 2018). The velocity imposed at the inlet is a function of time during a cough, and the flow field has the peak velocity v_{ip} (around 22.06 m/s) occurring at 6.60×10^{-2} s (Chao et al., 2009). The "trap" boundary condition is applied for all surfaces, i.e., the droplet will stay at the surface when it collides with the surface and then eliminate from the domain (Borro et al., 2021).

The pressure-based solver is employed as it is suitable for incompressible flows. The Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) algorithm is carried out as the pressure-velocity coupling method. We select first-order upwind for turbulence-related variables and second-order for other variables (such as pressure). The bounded second-order implicit formulation is the transient formulation, since it can bring a higher accuracy and better stability than others.

In the numerical simulation of a typical cough, when all droplets are integrated on the y-z plane, the positions of droplets at eight different times on the y-z plane (x = 0) are shown in Fig. 1. Different colors of droplets represent different diameters, which can be determined with the legend.

2. Sensitivity Analysis of α and β

Sensitivity analysis can identify the importance of input parameters in determining the value of an assigned output variable. There are mainly two approaches to analyzing sensitivity: Local Sensitivity Analysis, and Global Sensitivity Analysis. The former only focuses on the impact of one parameter on the calculation results, ignoring the interaction between parameters. However, the latter considers the influence of the whole parameter space on the results, and it can be further divided into qualitative (or screening) methods and quantitative methods. Qualitative sensitivity measures explore the relative importance of input variables affecting the output variable (e.g., Morris method), and quantitative analysis methods can obtain the quantified contribution of input parameters to the output parameter (e.g., Sobol method).

In general, when there are multiple parameters, qualitative measures are first used to conduct qualitative analysis on the parameters. Then, based on the results, parameters with high sensitivity are selected for further quantitative analysis. Here, only 2 parameters (α and β) need to be considered in the sensitivity analysis process, so the quantitative analysis methods are used directly. The widely used Sobol method is adopted here, which is a variance-based measure (Sobol, 2001). It can deal with nonlinear responses, and measure the effect of interactions in non-additive systems.

The total-effect index is used here as the evaluation identification, which measures the contribution to the output variance of the input variable, including all variance caused by its interactions, of any order, with any other input variables. The higher the value of total-effect, the higher contribution of the input parameter. Note that the sum of each parameters' total-effect will be greater than or equal to 1.00.

According to the previous results of personal exposure risk, the variation range of α is between 0.50 μg and 100.00 μg. Besides, β is set to change from 1.00×10^{-5} to 2.00×10^{-3} through numerous tests. Saltelli's sampling scheme generates

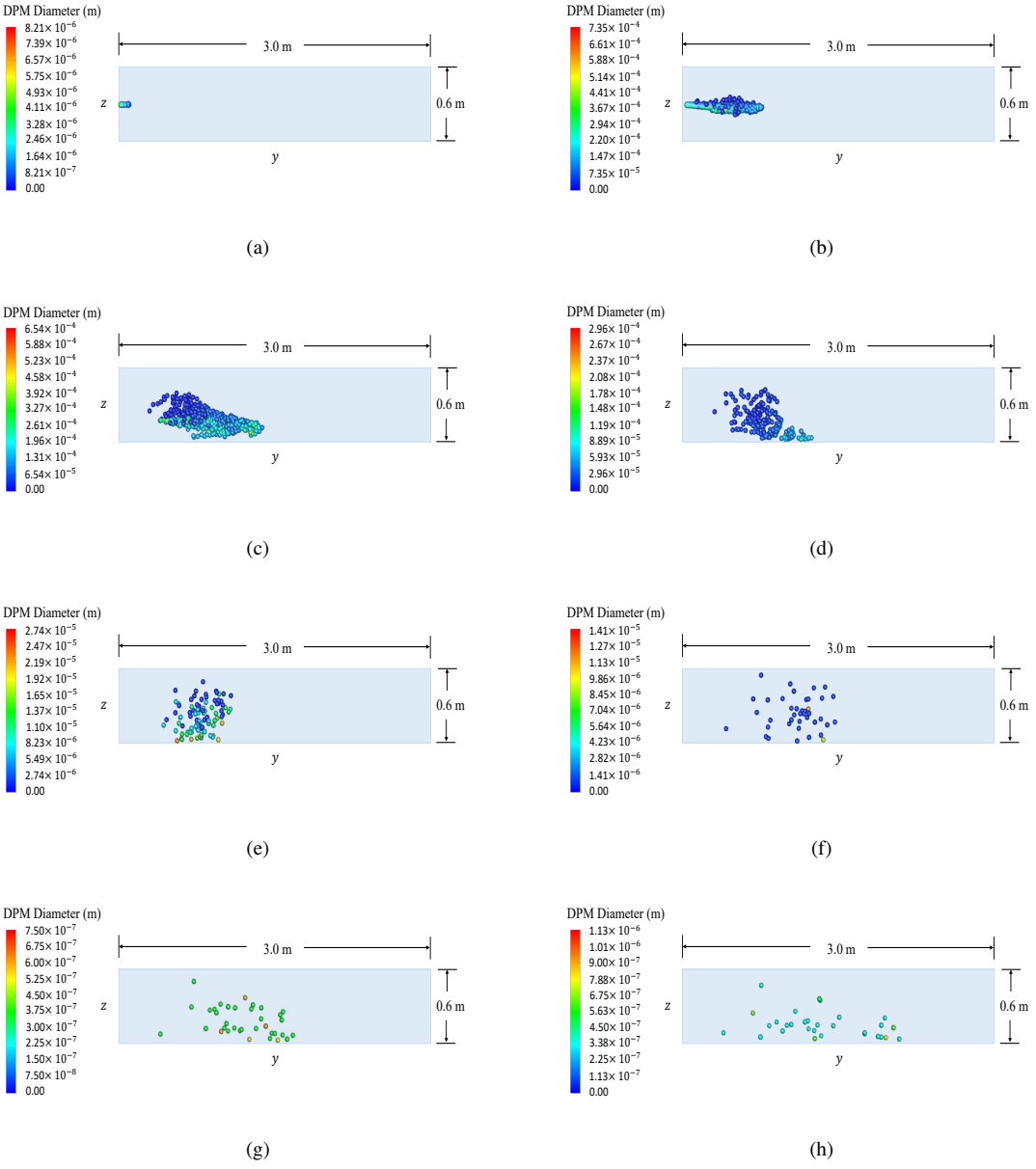

Fig. 1: Evolutions of the cough droplets' diameters in the computational domain on the y-z plane at different times: (a) 0.05 s; (b) 0.15 s; (c) 0.30 s; (d) 0.50 s; (e) 1.00 s; (f) 5.00 s; (g) 10.00 s; (h) 15.00 s.

6,000 samples for each training day. Based on the training set, all days' average total-effect of α and β are 0.986 and 0.269, respectively, where the confidence interval level is 95.00%. Results illustrate that the output C^{new} of our model depends on parameters α and β. Parameter α makes more contributions as expected because it is the cut-line of high exposure risk, which is the key to determining both the C^{risk} and C^{new}.

3. MAE Varies with α and β in Comparison Microscopic-level Models

In Xiao's model and Hernández-Orallo's model, MAE varies with α and β can be seen from Fig. 2 and Fig. 3. Following Equation (12) in the manuscript, there are $\alpha^* = 10.00$s and $\beta^* = 1.19\times10^{-4}$ in Xiao's Model (corresponding MAE is 7,205.67), and $\alpha^* = 0.60$ MEMs and $\beta^* = 1.41\times10^{-4}$ in Hernández-Orallo's Model (corresponding MAE is 7,172.78). Then, based on Equations (9-11) in the manuscript, the prediction results of the testing set by the two microscopic-level models are obtained.

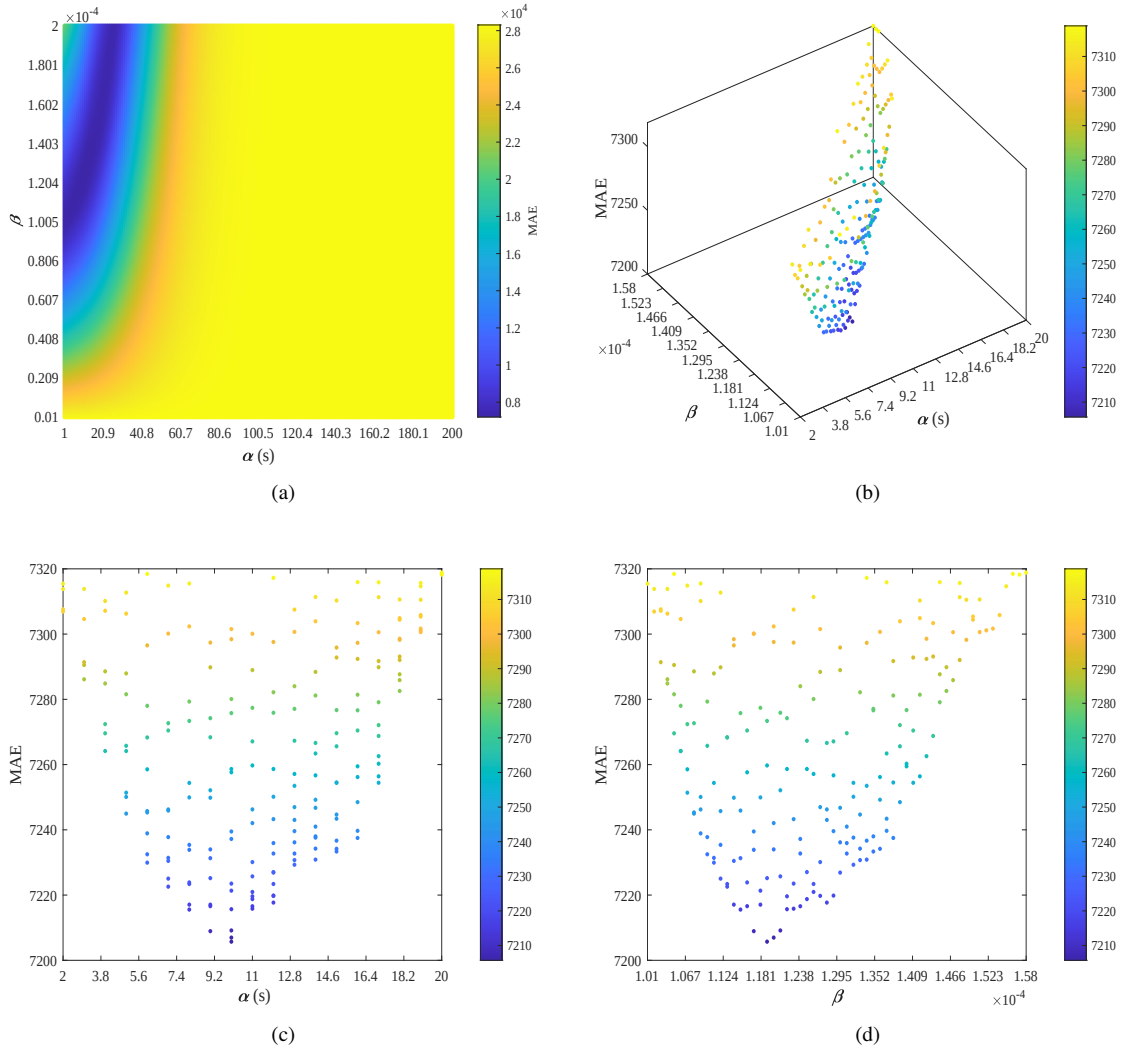

Fig. 2: MAE varies with α and β in Xiao's model: (a) the side view of $\alpha - \beta$ when $\alpha \in [1.00, 200.00]$ s and $\beta \in [1 \times 10^{-6}, 2 \times 10^{-4}]$; (b-d) the front view and 2 side views when MAE are less than 7,320.

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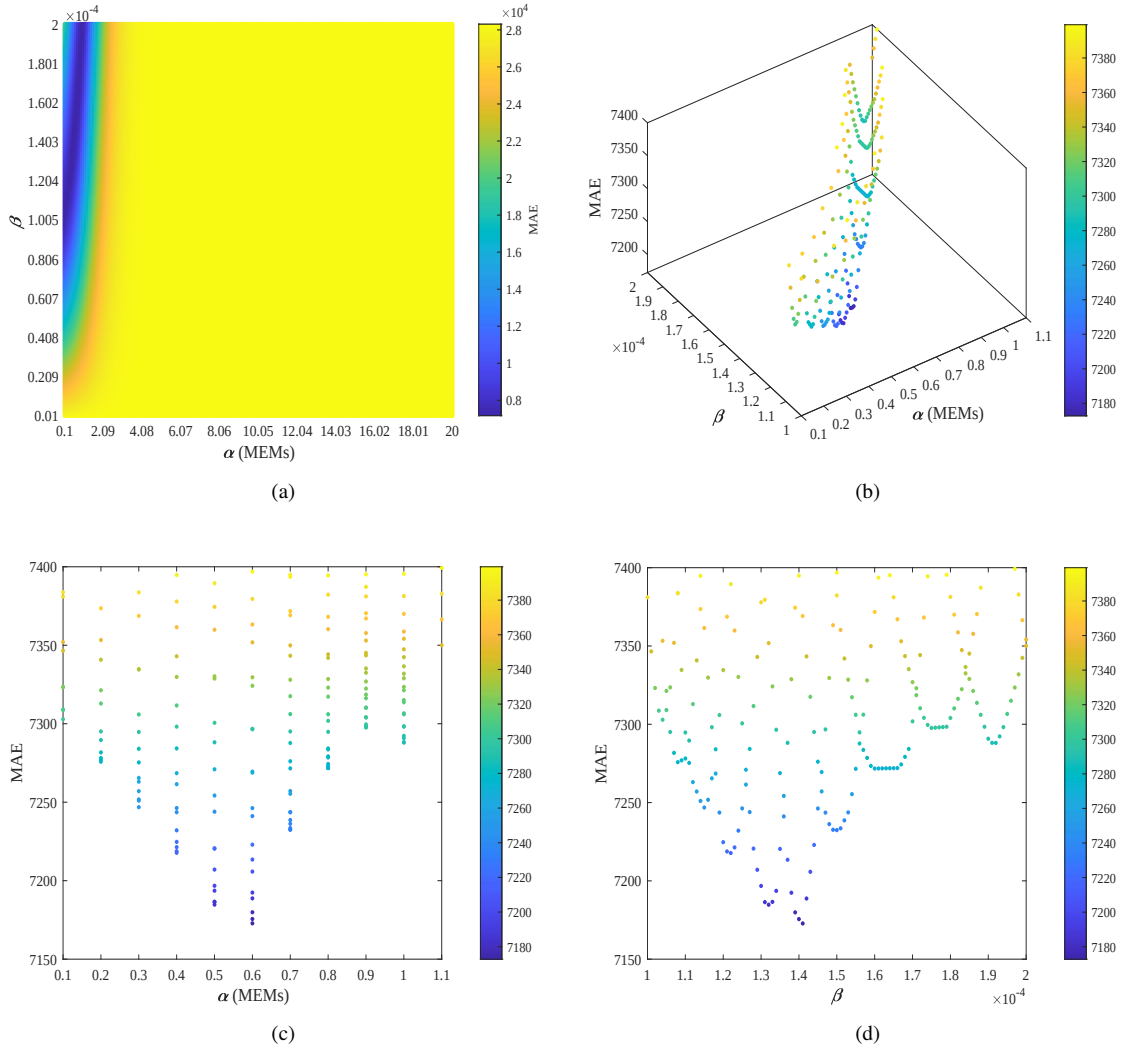

Fig. 3: MAE varies with α and β in Hernández-Orallo's model: (a) the side view of $\alpha - \beta$ when $\alpha \in [0.10, 20.00]$ MEMs and $\beta \in [1 \times 10^{-6}, 2 \times 10^{-4}]$; (b-d) the front view and 2 side views MAE are less than 7,400.